Cumidine

Other names:	1-Amino-4-isopropylbenzene
	4-(2-Propyl)aniline
	4-Amino-1-isopropylbenzene
	4-Aminocumene
	4-Isopropylaniline
	Aniline, p-isopropyl-
	Benzenamine, 4-(1-methylethyl)-
	Cumene, p-amino-
	NSC 7198
	p-Cumidine
	p-Isopropylaniline
	«beta»-(4-Aminophenyl)propane
	Â«betaÂ»-(4-Aminophenyl)propane
Inchi:	InChI=1S/C9H13N/c1-7(2)8-3-5-9(10)6-4-8/h3-7H,10H2,1-2H3
InchiKey:	LRTFPLFDLJYEKT-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CC(C)c1ccc(N)cc1
Mol. weight [g/mol]:	135.21
CAS:	99-88-7

Physical Properties

Property code	Value	Unit	Source
gf	191.69	kJ/mol	Joback Method
hf	24.48	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	48.82	kJ/mol	Joback Method
ie	7.70 ± 0.10	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.392		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1200.00		NIST Webbook
tb	498.20	K	NIST Webbook
tc	734.84	K	Joback Method
tf	298.39	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.79	J/mol×K	509.07	Joback Method
cpg	285.89	J/mol×K	546.70	Joback Method
cpg	299.13	J/mol×K	584.33	Joback Method
cpg	311.56	J/mol×K	621.96	Joback Method
cpg	323.20	J/mol×K	659.58	Joback Method
cpg	334.09	J/mol×K	697.21	Joback Method
cpg	344.26	J/mol×K	734.84	Joback Method
hvapt	57.50	kJ/mol	416.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	499.70	K	99.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48264e+01
Coeff. B	-4.27271e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	373.52
Temperature range (K), max.	528.69

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99887&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume